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Invited Article

Modelling Scenario in Nanotechnology Today

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Abstract

This paper focuses on the current scenario of Nanotechnology vis-a-vis the latest progress and developments in the field in the last decade from a modelling and computational viewpoint. The importance of incorporating better and faster modelling and simulation tools not only in the multiscale context but also from a predictive point of view for future technological discoveries and innovations is also discussed. Challenges in this arena and priorities for the next decade are also discussed.

Keywords: Computational Nanotechnology, Modelling and Simulation

1. INTRODUCTION

Even though Nanotechnology has long been considered by many as a diehard experimental discipline, it has attained the profound status of a new realm of science and technology only with the backing of a deep understanding of the physics of the micro and nanoworld and its dynamics followed by strong computational backing with the support and advent of fast computers and new technologies. This paper makes an attempt to visualize the effort and impact of computational theory, modelling and simulation that has been incorporated in Nanotechnology over the years and critically examines not only the wealth of ideas and information accumulated over the years with a modelling perspective, but tries to make a projection of trends and offers creative ideas for new initiatives vis-a-vis the possible vision of what the technology with a computational backing could mean in the years to come.

Enormous investments have been made in nanotechnology research and according to Cientifica's2011 released report on Global Nanotechnology Funding and Impact, in the last 11 years, Governments around the world have invested more than US \$67.5 billion in nanotechnology funding. Taking into account, corporate research and various other forms of private funding, nearly a quarter of a trillion dollars will have been invested in nanotechnology by around 2015. Most of this research in nanotechnology, however, is still done by expensive and time consuming experiments on the one hand whereas industry demands faster and less expensive solutions. Modelling and design simulation of materials seems to be the only way to address this challenge.

2. ADVANCES IN THE LAST DECADE

The term 'Nanotechnology' first introduced by a Japanese engineer Norio Taniguchiin 1974 (Taniguchi, 1974), originally implied a technology that went beyond controlling materials and engineering on the micrometer scale which had dominated the twentieth century. Today, however, the word has undergone a metamorphosis in meaning and relates more to the visionary view of Eric Dexler (Eric Dexler, 1986) where at the nanometer length scales, Nanotechnology corresponds more to the atom-by-atom manipulative, hardtech pressing methodology where many diverse enabling and associated technologies begin to coalesce.

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With rapid development seen over the past decade, researchers now have been able to gain substantial control over particle size, crystal shape, structural phase and chemical and physical properties of many materials. Further, improved computational capacity has helped in the understanding of this process phenomena in a greater depth through theoretical investigation and computer simulation and has allowed us to exercise a complete control over the structure and functioning of physical matter, a control that implies that physical matter can be interrogated atom-by-atom and molecule-by-molecule so that new forms of materials and devices can be designed by a precise positioning of individual atoms and thereby can operate at highly reduced length, time and energy scales[3].

Theory, Modelling and Simulation have played a crucial, supportive and many times even a critical role in the many advances seen in Nanotechnology in the last decade [4]. New theoretical ideas gave birth to new modelling approaches as well as advent of powerful computational capabilities permitted larger and more complex problems like multiscale modelling to be addressed, which resulted in the effective delivery of complex simulations being expressed in a language used by experimentalists and designers. To showcase a few,

- Advances in *ab initio* theory beyond density functional theory(Quek et al. 2009)
- Advances in linear-scaling quantum mechanics (Niklasson, 2002) (Wang et al. 2008)
- New statistical theories for conduction in carbon nanotubes and semiconductor nanowire networks (Cao et al. 2008;Cao et al. 2009)
- Development of non-equilibrium Green's function approach as a conceptual and computational for describing quantum transport with practical applications in molecular electronics (Datta 2005) (Quek et al. 2007)
- Understanding of the current flow at the molecular scale (Venkataraman et al. 2006a; Quek et al. 2007; Quek et al. 2009)
- Evolution of microelectronics into nanoelectronics (Lundstrom and Ren 2002)
- Discovery of grapheme and carbon-based electronics (Javey et al. 2003; Heinze et al. 2002; Cao et al. 2008;Cao et al. 2009)
- Discovery of iron-based High T_c Superconductors (Kamihara et al. 2008; Maier et al. 2008)
- Ten orders of magnitude improvement in the sensitivity of biosensors (Li et al. 2004; Li et al. 2005; Star et al. 2006; Nair and Alam 2006; 2007)

All the above coupled with the fact of significant advances in computing,highlight the increasing role of modelling and simulation in nanotechnology where a stage seems to have been set up for an even more ambitious agenda for theory, modelling and simulation in nanotechnology in the days to come.

3. CHALLENGES AND PRIORITIES IN THE NEXT DECADE

Multiscale Modelling and Simulation provides investigative tools to support nanotechnology by developing new conceptual and modelling frameworks. To make them more effective they should be able to solve larger problems more accurately and efficiently. This is the key that can transform research by identifying promising ideas and convert them in to real technologies, bring about meaningful technology development thereby creating better designs and utilitarian products. Important barriers that need to be crossed in the future are highlighted below.

- Need to develop a strong long-term dialogue between different disciplines spanning nanoscience and engineering. Experts need to acquire knowledge from experts in other fields and people involved in theory, modelling and simulation need to connect with experimentalists and device designers to seek solutions to common problems
- To realize the transformative potential of nanotechnology, educators need to devise efficient programs that truly integrate different disciplines

from a nano perspective so as to create students with a depth of knowledge in a single discipline in addition to making them useful contributors to multidisciplinary teams

- Need to train a new generation of computational nonscientists with expertise in advanced, numerical algorithms, parallel computing and shrewd enough to exploit the latest characteristics of new generation computing technology.
- Need for testing and validating databases as well as disseminating new research methods and software
- Need for workforce development and in-service training with efficient, affordable and open-source technology transfer of computational tools from academia to industry and vice-versa.

4. CONCLUSION

Predictive modelling and simulation in nanotechnology will not only create a supporting role in nanoscience understanding but seems to be poised to play a determinative and leading role in the next ten years with a potential to accelerate research and development in nanotechnology with substantial impact on society. Futuristic modelling and simulation coupled with powerful human interfaces can create great results both academically and pedagogically that can redefine educational paradigms and impact science students at all levels thus addressing the challenges that human society faces in energy, environment, health and security.

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